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Si-C atomic bond and electronic band structure of a cubic $Si_{1-y}C_y$ alloy

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We apply the sp^3s^* tight-binding model to study the electronic energy band structure of the cubic $Si_{1-y}C_y$ alloy. First by the effective medium approximation where local atomic fine structures are averaged out, it is obtained that the energy band gaps of both relaxed and strained $Si_{1-y}C_y$ alloys increase with increasing C content. The effect of the local Si-C atomic bond structure on the energy band is studied in the real space in order to include the actual broken translational symmetry in the $Si_{1-y}C_y$ alloy. The electronic local densities of states are investigated and the following is concluded: (a) When Si-C bond length in the alloy assumes the crystal SiC one (strained alloy), an electronic state at the C atom and its surrounding Si atoms is induced in the energy band gap of crystal Si. The valence band edge is slightly lifted. The results indicate a type I energy band alignment for strained $Si_{1-y}C_y/Si$ quantum well. (b) When the Si-C bonds assume the Si-Si bond length of the crystal Si (relaxed alloy), the electronic states are not much modified. [S0163-1829(98)07535-3]

I. INTRODUCTION

The realization of many kinds of electronic and optoelectronic devices in strained layer $Si_{1-x}Ge_x/Si$ heterostructures has stimulated a great interest in investigating IV-IV binary and ternary alloys.[1,2] However, the strained epitaxial $Si_{1-x}Ge_x$ layers without misfit dislocations can be grown on a Si substrate only by a low-temperature growth technique.[1] Moreover, the application of $Si_{1-x}Ge_x/Si$ materials is restricted by the strain in the epilayers.

To compensate the strain, C atoms with an atomic diameter smaller than the ones of both Si and Ge atoms are introduced into the Si-Ge system to form $Si_{1-x-y}Ge_xC_y$ alloys. The substitutional C atoms in $Si_{1-y}C_y$ and related alloys also offer an additional parameter for tailoring the energy band structure.[2] The investigation on $Si_{1-y}C_y$ and related alloys is thus of great importance to understand the band-gap engineering for Si-based semiconductor materials.

Recently, $Si_{1-y}C_y$ and related alloys with substitutional C atom composition above 1% have been experimentally obtained on Si substrates by low-temperature growth techniques (although carbon bulk solubility in Si is only about 10^{-4}% at the melt point).[3,4] Many efforts, both theoretical and experimental, have been performed to characterize the energy band structure of $Si_{1-y}C_y$ and related alloys.[2,4–7] So far the understanding of the electronic energy band structures of such materials is limited.

In 1983 Vogl, Hjalmarson, and Dow published their results of a sp^3s^* nearest-neighbor semiempirical tight-binding theory of energy bands in zinc blende and diamond structure materials.[8] The theory was developed from the sp^3 tight-binding model of Harrison.[9] In this work we shall study the electronic energy band structure of the cubic $Si_{1-y}C_y$ alloy based on this model.

As compared with early theoretical studies, e.g., Refs. 10 and 11, the present study shall focus on the microstructures of the Si-C bond and its surrounding Si-Si bonds in the alloy that lacks the translational symmetry. Because of the lack of the translational symmetry, we shall perform the numerical investigation in the real space.

The theoretical investigation is divided into two parts. We present in Sec. III the results based on the effective medium approximation. The local environment effects are the focus of the work. Due to the broken translational symmetry in the alloy the local Green's function theory is applied in Sec. IV to study the dependence of the local density of energy states on the Si-C atomic bond structure. Discussions and summary are made in Sec. V.

II. ENERGY BAND STRUCTURE OF $Si_{1-y}C_y$ ALLOY AT SMALL *k*

Because we concentrate on the $Si_{1-y}C_y$ alloy with low C content, the diamond crystal lattice structure is assumed for the alloy here.

As developed by Vogl, Hjalmarson, and Dow,[8] we introduce five Löwdin orbitals, $|s\rangle$, $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$, and $|s^*\rangle$, at each atomic site $\mathbf{r}_i$. The Hamiltonian matrix element is denoted as $h(\alpha\beta,ij)$ between the αth orbital on the ith atomic site $|\alpha,i\rangle$ and the βth orbital on jth site $|\beta,j\rangle$, where either $i=j$ or i is a nearest neighbor of j. The values of these matrix elements are listed in Table I for crystal Si, C, and SiC.[8] In Table I the diagonal elements are denoted as E (orbital energies), and the off-diagonal elements are V (interaction energies).

In Ref. 8, the top of the valence band, $\Gamma_{15}^{v}=0$, is the reference energy for every individual material. Referring to the C energy band, an energy band offset between C and SiC, $\epsilon(\mathrm{SiC})=\Gamma_{15}^{v}(\mathrm{SiC})-\Gamma_{15}^{v}(\mathrm{C})$ is to be added to the SiC orbital energies. Similarly, an energy band offset $\epsilon(\mathrm{Si})=\Gamma_{15}^{v}(\mathrm{Si})-\Gamma_{15}^{v}(\mathrm{C})$ is to be added to the Si orbital energies. From available values [the electron affinity of diamond is

TABLE I. Energy band structure parameters for the sp^3s^* tight-binding band calculation.

	Si	C	SiC
$E(s,a)$	-4.2000	-4.5450	-8.4537
$E(p,a)$	1.7150	3.8400	2.1234
$E(s^*,a)$	6.6850	11.3700	9.6534
$E(s,c)$	-4.2000	-4.5450	-4.8463
$E(p,c)$	1.7150	3.8400	4.3466
$E(s^*,c)$	6.6850	11.3700	9.3166
$V(s,s)$	-8.3000	-22.7250	-12.4197
$V(x,x)$	1.7150	3.8400	3.0380
$V(x,y)$	4.5750	11.6700	5.9216
$V(sa,pc)$	5.7292	15.2206	9.4900
$V(sc,pa)$	5.7292	15.2206	9.2007
$V(s^*a,pc)$	5.3749	8.2109	8.7138
$V(pa,s^*c)$	5.3749	8.2109	4.4051
a [Å]	5.431 (Ref. 12)	3.566 (Ref. 12)	4.360 (Ref. 12)
Affinity	4.05	2.3 (Ref. 14)	4.29 (Ref. 13)
Bandgap	1.12	5.50	2.2

very substrate-orientation dependent,[14] a value of 2.2 eV is obtained for (001) orientation] it is easy to obtain the absolute positions of valence band edges (Γ_{15}^{v}) below the vacuum level: 5.17 eV for Si, 6.49 eV for SiC, and 7.8 eV for C. Thus, $\epsilon(\mathrm{SiC})=1.31$ and $\epsilon(\mathrm{Si})=2.63$ eV.

For a $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy, the interaction elements are obtained by the well-known d^{-2} scaling rule.[9]

The eigenfunction of the system is expressed by

$$\sum_{\alpha,i} C(\alpha,i)|\alpha,i\rangle.$$

The coefficients in the above linear combination satisfy the eigenvalue equation

$$\sum_{\beta,j} h(\alpha\beta,ij)C(\beta,j)=EC(\alpha,i). \tag{1}$$

For crystals Si, C, and SiC, we apply the Fourier transformation

$$\begin{aligned} C(\alpha,\mathbf{k})&=\frac{1}{\sqrt{N}}\sum_i C(\alpha,i)\exp(i\mathbf{k}\cdot\mathbf{r}_i),\\ H(\alpha\beta,\mathbf{kq})&=\frac{1}{N}\sum_{ij} h(\alpha\beta,ij)\exp[i(\mathbf{k}\cdot\mathbf{r}_i-\mathbf{q}\cdot\mathbf{r}_j)]. \end{aligned} \tag{2}$$

Equation (1) reduces to

$$\sum_{\beta,\mathbf{q}} H(\alpha\beta,\mathbf{kq})C(\beta,\mathbf{q})=E(\mathbf{k})C(\alpha,\mathbf{k}). \tag{3}$$

Here N is the number of atoms in the system.

Because of the translational symmetry,

$$\begin{aligned} h(\alpha\beta,ij)&=h(\alpha\beta,\mathbf{r}_i-\mathbf{r}_j)\\ H(\alpha\beta,\mathbf{kq})&=\delta_{\mathbf{k},\mathbf{q}}H(\alpha\beta,\mathbf{k})\\ &=\delta_{\mathbf{k},\mathbf{q}}\sum_{ij} h(\alpha\beta,ij)\exp[i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)],\\ &\times\sum_{\beta} H(\alpha\beta,\mathbf{k})C(\beta,\mathbf{k})=E(\mathbf{k})C(\alpha,\mathbf{k}). \end{aligned} \tag{4}$$

In a $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy, $h(\alpha\beta,ij)$ is not invariant with respect to lattice translations, Eqs. (4) are thus not valid. However, let us approximate $h(\alpha\beta,ij)$ by its mean value in the limit of long wavelength (small $|\mathbf{k}|$). In this case, the term $\exp[i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}_j)]$ in Eq. (2),

$$\exp[i(\mathbf{k}\cdot\mathbf{r}_i-\mathbf{q}\cdot\mathbf{r}_j)]=\exp[i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)]\exp[i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}_j)], \tag{5}$$

can be approximated as constant over a large area of the structure (effective-medium approximation). Let

$$h'(\alpha\beta,ij)=\frac{\Sigma_{mn}h(\alpha\beta,mn)\delta_{\mathbf{r}_m-\mathbf{r}_n,\mathbf{r}_i-\mathbf{r}_j}}{\Sigma_{mn}\delta_{\mathbf{r}_m-\mathbf{r}_n,\mathbf{r}_i-\mathbf{r}_j}}, \tag{6}$$

which is invariant under lattice translations, we then have

$$H'(\alpha\beta,\mathbf{kq})\approx\frac{1}{N}\sum_{ij} h'(\alpha\beta,ij)\exp[i(\mathbf{k}\cdot\mathbf{r}_i-\mathbf{q}\cdot\mathbf{r}_j)], \tag{7}$$

and

$$\begin{aligned} H'(\alpha\beta,\mathbf{kq})&=\delta_{\mathbf{k},\mathbf{q}}H'(\alpha\beta,\mathbf{k})\\ &=\delta_{\mathbf{k},\mathbf{q}}\sum_{ij} h'(\alpha\beta,ij)\exp[i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)],\\ &\times\sum_{\beta} H'(\alpha\beta,\mathbf{k})C(\beta,\mathbf{k})\\ &=E(\mathbf{k})C(\alpha,\mathbf{k}). \end{aligned} \tag{8}$$

The above equations are mathematically identical to Eqs. (4). It must be recalled that the solutions are valid only when $|\mathbf{k}|$ is small. The approximation is generally acceptable for the valence band top at Γ_{15}^{v}, while for the conduction band edge of an indirect band gap material like Si, more sophisticated theoretical treatment is required.

When the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy is grown on a Si substrate, it is strained when the layer is thin. The atomic bond length is uniform and fixed by the substrate Si; the atomic bonds become relaxed when the layer becomes thicker. In the effective-medium approximation, the lattice constant of the relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy is obtained by linear interpolation between bond lengths of C and SiC when $y>0.5$, it is obtained from SiC and Si when $y<0.5$.

Figure 1 shows the energy dispersion relations of relaxed and strained $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloys as functions of the C mole fraction y. The positions of the conduction and valence-band edge are plotted in Fig. 2 as functions of the C content. The wave vector k_c corresponding to the conduction-band minimal along the X direction is also presented in Fig. 2.

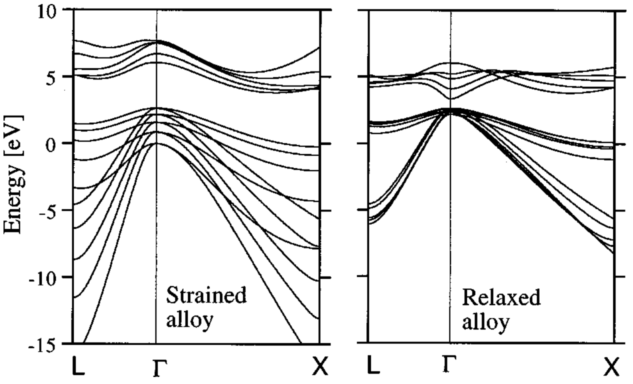

FIG. 1. The energy dispersion relations of relaxed and strained $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloys. $y=0$, 0.25, 0.50, 0.75, 1.0.

For a strained $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy, both the valence and conduction bands are vertically shifted along the energy axis following the increase of the C mole fraction. The band gap is indirect and increases monotonically with the C mole fraction.

On the other hand, the valence band of a relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy is not much affected by the C mole fraction. The band gap of relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy is indirect and increases with increasing y when $y<0.35$. However it becomes a direct-band-gap material when $y>0.35$. The energy band gap increases with increasing y from 0 to 0.35, then decreases when increasing y from 0.35 to 0.5. After that, the energy band gap increases again with y.

Let us check the validity of the conclusion that the energy band gap increases with increasing but small y. It is easy to see that Eq. (6) can be rewritten as

$$h'=(1-y)h_{\mathrm{Si}}+yh_{\mathrm{SiC}} \tag{9}$$

for small y value, where h_{Si} and h_{SiC} are interaction elements in crystal Si and SiC, respectively. Since the energy band gap is proportional to the interaction elements, the above equation indicates an increasing energy band gap of $\mathrm{Si}_{1-y}\mathrm{C}_y$ as a function of the C content (the band gaps of C and SiC are wider than the Si one). It is thus observed that the conclusion of increasing band gap with y is very general, even when we are working with the relatively simple sp^3s^* tight-binding model.

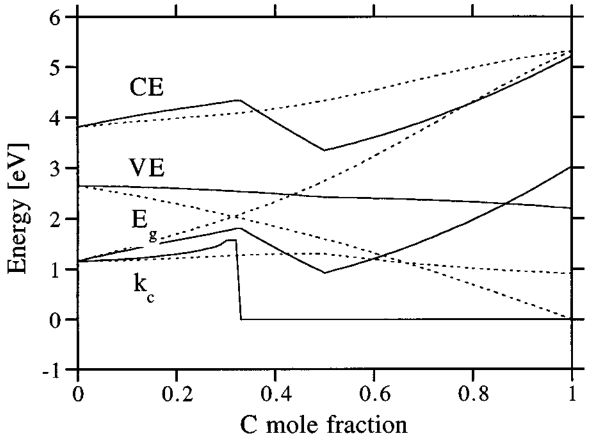

FIG. 2. The conduction- and valence-band edges CE and VE, the energy band gap E_g, and the wave vector of minimal conduction band edge k_c of relaxed (solid lines) and strained (dotted lines) $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloys.

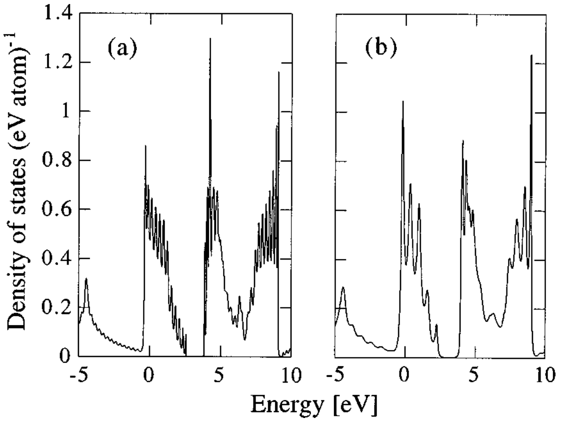

FIG. 3. The density of states of the crystal Si calculated by (a) 120 pairs of (a,b) coefficients; (b) 50 pairs of (a,b) coefficients.

It must be emphasized that the conclusions thus obtained from Eqs. (8) about the valence-band edge (Γ_{15}^{v}) are generally valid since they are obtained in consistence with the presumption of small $\mathbf{k}$. The results about the conduction-band edge of the relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy may also be valid when $y>0.35$, since the result indicates a direct band-gap material with a conduction-band edge at $\mathbf{k}=0$. The results about the conduction-band edges at finite $\mathbf{k}$ are to be examinated.

To study more elaborately the conduction-band edge of the indirect-band-gap $\mathrm{Si}_{1-y}\mathrm{C}_y$ materials, we present in the following section our further theoretical investigations, which take into account the broken translational symmetry in the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy.

III. LOCAL ATOMIC BOND EFFECT ON ENERGY BAND STRUCTURE

Generally speaking, in a $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy, except for the restriction of the compositional parameter y, each atomic site can be occupied by either a Si atom or a C atom. The system thus lacks the translational symmetry, which is the basis for wave-function expansion in $\mathbf{k}$ space. Equation (1) has to be solved in real space. Many numerical methods have been developed to study the electronic energy band structure in real space. Among them is the recursion method developed by Haydock, Heine, and Kelly,[15] which is well suited here for the study of the local environment effects.

The recursion method constructs a new set of normalized orthogonal basis, in which the general Hamiltonian matrix is turned into a tridiagonal form, the diagonal elements of the corresponding local Green's function matrix is expressed as continued fractions of the diagonal and off-diagonal elements, (a,b) of the tridiagonalized Hamiltonian matrix, from which the local densities of states are obtained. The method has been successfully applied to various systems.[16]

In Fig. 3 we present the calculated density of states of the crystal Si using an atomic cluster of 100 149 atoms and a cluster with 1 422 260 atoms, corresponding to 50 and 120 pairs of diagonal and off-diagonal (a,b) coefficients, respectively. The computer RAM requirement to calculate 120 (*a*,*b*) pairs is more than 256 Mb, the upper limit of our computation capability. Here we see a much more accurate band edge determination by 120 pairs of (*a*,*b*) than the one by 50 pairs. The numerical fluctuations in the calculated density of states are induced by the limited space that can be involved. There have been attempts to solve this problem.[16] Many methods use the oscillation properties of (*a*,*b*) as functions of *n* to extrapolate (*a*,*b*) to much larger *n*. However, the methods are not valid here since we are discussing random systems. We identify the peaks and band edges from artificial numerical fluctuations in the local densities of states by comparing local densities of states calculated from 50, 100, and 120 pairs of (*a*,*b*) coefficients.

Because of the energy band offset, the valence-band edge of the Si is shifted to 2.6300 eV. A peak in the density of states is clearly observed at 3.8725 eV below the main conduction band. The 3.8725-eV peak is identified as the conduction-band minimal at k_c. The energy band gap of the crystal Si thus calculated is 1.1205 eV.

Because of the extremely low C content in the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy usually studied experimentally, the C atoms in the alloy are approached as uniformly distributed with negligibly small correlation among them. In theoretical investigations, the spatial positions of the C atoms in the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy can be generated by random numbers in the computers. We concentrate on a system of the crystal Si in which the central Si atom has been substitutionally replaced by a C atom.

The averaged lattice constant of our relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy is almost the same as the crystal Si because of the low C content. The orbital energies of the central C atom assume the ones of the C atom in crystal SiC. The interaction strengths of the Si-C bonds assume the ones in crystal SiC if their bond lengths are the same. Otherwise, the d^{-2} scaling rule applies. We consider the following two different Si-C bond lengths.

First we shall consider that the Si-C bond lengths in the alloy are the same as in the crystal SiC's. The lattice mismatch thus induced between the central C atom and its four nearest-neighbor Si atoms applies on the bonds between the 4 first-nearest-neighbor Si atoms and 12 second-nearest-neighbor Si atoms. This corresponds to a local strained $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy. (From the experimental point of view, a strained film means that the epilayer has the same lattice constant as the substrate on which the film has been deposited, a relaxed epilayer has the same lattice constant as that of the bulk crystal with identical composition.) Figure 4(a) shows the local density of states of the central substitutional C atom in such a strained $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy.

We see here that the energy band structure has been drastically modified by the strain. The valence-band edge at the C atom moves into the energy band gap of the crystal Si and an electronic state indicated by an arrow in Fig. 4(a) in the energy band gap is clearly observed in the local densities of states, not only at the C atom, but also at its surrounding Si atoms.

The local environment effects are presented in Figs. 4(b) and 4(c) [see also Figs. 5(b) and 5(c)] where the local densities of states of the Si atoms of the first and second nearest neighbors to the central C atom are calculated. The density of states of the crystal Si is plotted as Fig. 4(d) for comparison. It is shown that the introduction of the central C atom affects mainly the local energy band structure of C atom itself and its first nearest-neighbor Si atoms as compared with the crystal Si.

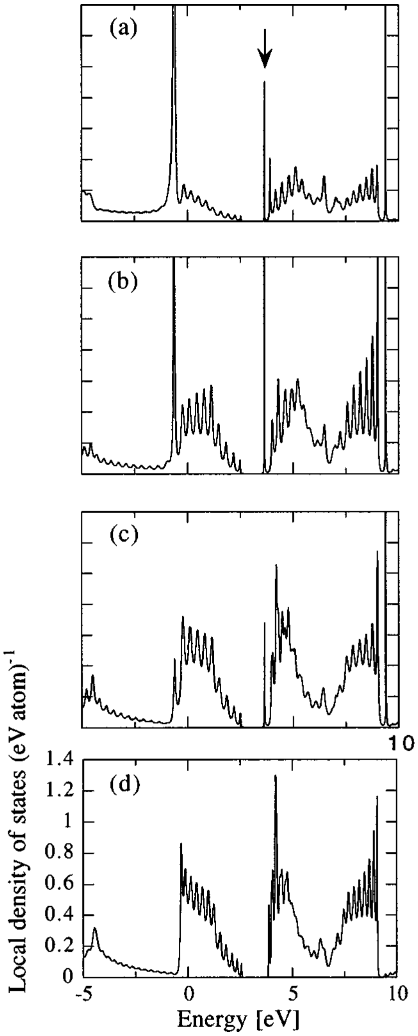

FIG. 4. The local density of states of (a) the substitutional C atom, (b) the first- and (c) the second-nearest-neighbor Si atoms, when the Si-C bond lengths assume the Si-C bond lengths in crystal SiC (macroscopically strained $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy). (d) is the density of states of crystal Si for comparison.

The changes of the valence band edge from the C atom to the neighboring Si atoms and the crystal Si are continuous. However, the position of the electronic state below the conduction band edge of the crystal Si is constant in the C atom and its surrounding Si atoms, indicating an electronic quasilocal state.

Figure 5(a) shows the calculated local density of states at the central C atom when the system has the second type of Si-C bonds, namely, the bond lengths in the system are uniform as the Si-Si bonds in the crystal Si, which corresponds to a macroscopically relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy. Figure 5 indicates that the energy band structure is not greatly affected by such a substitutional C atom.

Because the changes in the local densities of states induced by the substitutional C atom are rather local, the total density of states of the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy can be approximated as

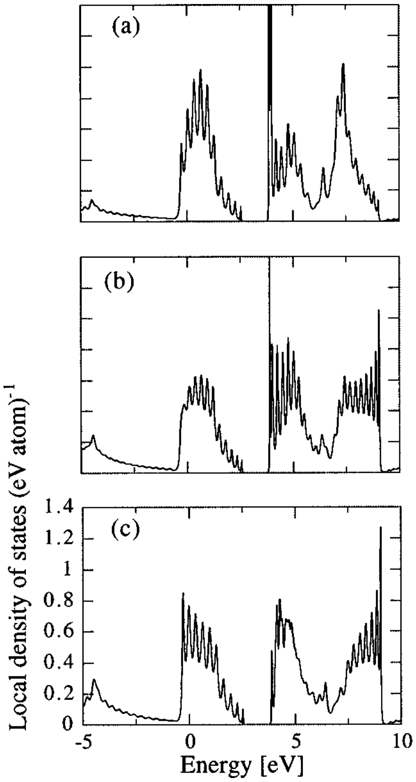

FIG. 5. Same as Fig. 4 but for the cases when the Si-C bond lengths assume the Si-Si bond lengths in crystal Si (macroscopically relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy).

$$\nu=\frac{y}{5}\,(\nu_{\mathrm{C}}+\nu_1+\nu_2+\nu_3+\nu_4)+(1-y)\,\nu_{\mathrm{Si}}, \tag{10}$$

where ν_{C} is the local density of states of the central C atom, ν_i, $i=1,2,3,4$, are the ones of the four first-nearest-neighbor Si atoms, and ν_{Si} is the density of states of the crystal Si.

It is concluded by the above equation that the energy band gap of the strained $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy decreases with an increasing C mole fraction (it is reminded here that we are investigating the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy with small C content). A type I energy band alignment for possible $\mathrm{Si}_{1-y}\mathrm{C}_y/\mathrm{Si}$ quantum wells is expected by Fig. 4. The narrowing of the energy band gap of the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy has been reported experimentally. A type I band alignment was measured in $\mathrm{Si}_{1-y}\mathrm{C}_y/\mathrm{Si}$ quantum wells recently and the redshift of the band edge related photoluminescence has been observed from a high-quality pseudomorphic $\mathrm{Si}_{1-y}\mathrm{C}_y$ layer in $\mathrm{Si}_{1-y}\mathrm{C}_y/\mathrm{Si}$ quantum well structures.[17,18] When the C-Si bonds assume the Si-Si bond length in the crystal Si, a slightly modified energy band structure is observed in Fig. 5 for the relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy.

It is important to note that stretched Si-C bonds (strained as compared with the corresponding bond length in crystal SiC) indicate uniform atomic bond length and thus a relaxed alloy; spatial variation in the lattice constant, and thus strained alloy, arise when the Si-C bonds become relaxed with respect to the crystal SiC on the other hand.

The modification of the energy band by strain can be qualitatively described by the general d^{-2} scaling law: The interaction strength of the Si-C bond with a crystal Si-Si bond length is closer to the one in the crystal Si than is the Si-C bond with a crystal SiC bond length. For example, for $V(sc,pa)$ the relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy is $(4.36/5.43)^2 \times 9.2007=5.932$ eV, as compared with 5.73 eV in the crystal Si. It is 9.2007 eV for the strained $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy, which naturally results in a much affected local density of states in Fig. 4. Here again we see that our conclusions are quite general. They do not depend on the special tight-binding model we are working with.

IV. CONCLUSIONS AND DISCUSSIONS

We have applied the sp^3s^* tight-binding model to study the energy band structure of the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy. It has been discussed, however, that our conclusions about the electronic energy band structure of the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy in general do not depend on this specific tight-binding model.

We have first used an effective-medium approximation to study the outline of the energy band structure of the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy. In this approach all the details concerning local atomic bonds are averaged out. For a strain relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy, it is found that the band structure changes with varying C composition in the alloy. The relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy is an indirect band material and the band gap increases with the increasing C composition when $y<0.35$. The alloy becomes a direct band semiconductor and the band gap decreases with the increasing C content when $y>0.35$. The band gap increases again after reaching a minimum at $y=0.5$. For the strained $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy, the energy band is indirect and the band gap monotonously increases with the increasing C composition.

In order to describe accurately the local atomic bond structure and its effect on the energy band structure of the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy, we studied the local densities of electronic states in real space considering the broken translational symmetry in the alloy. For the strain relaxed $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy, it is found that the energy band structure is hardly modified by the substitutional C atoms.

However for locally strained $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy, the energy band gap decreases with increasing C content. Such band-gap shrinking, different from the prediction of the effective-medium approximation, is due to the local strain around the substitutional C atoms, which are randomly distributed in the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy.

The results indicate the vital importance of the local atomic bond structure in studying the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy. By the effective-medium approximation, all the local fine structures are completely averaged out, the band gap of the $\mathrm{Si}_{1-y}\mathrm{C}_y$ alloy increases linearly with the C mole fraction when y is small, which is normally expected by the presumptions in the effective-medium approximation.

We have neglected the correlation among C atoms in the alloy. In addition we have applied the sp^3s^* tight-binding model, which neglects many physical phenomena, e.g., the spin-orbit interactions that are very important in Si and Si-related materials. Moreover, when calculating or observing the band gap change induced by the incorporation of C atoms, one should be careful to distinguish the substitutional and interstitial C in $\mathrm{Si}_{1-y}\mathrm{C}_y$ and related alloys because of the difficulty in introducing substitutional C into Si and the effect of interstitial C on the band gap.[19] Further investigation about these important factors is in progress.

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